

08/30/2006 10776946.trn

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NEWS 16 AUG 09 INSPEC enhanced with 1898-1968 archive
NEWS 17 AUG 28 ADISCTI Reloaded and Enhanced
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FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 29 AUG 2006 HIGHEST RN 905300-98-3
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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

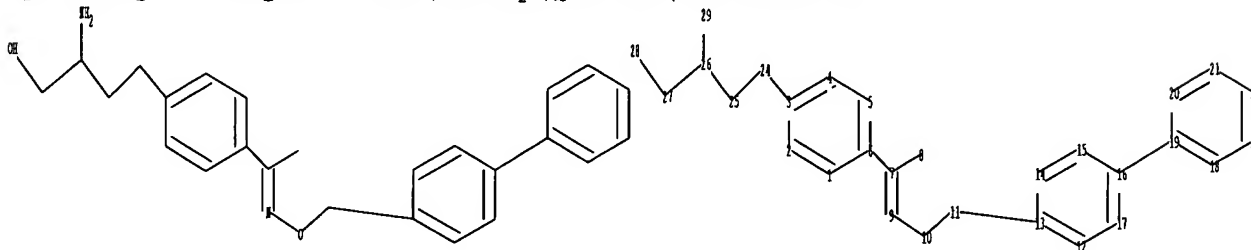
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<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10776946.str



08/30/2006 10776946.trn

chain nodes :

7 8 9 10 11 24 25 26 27 28 29

ring nodes :

1 2 3 4 5 6 12 13 14 15 16 17 18 19 20 21 22 23

chain bonds :

3-24 6-7 7-8 7-9 9-10 10-11 11-13 16-19 24-25 25-26 26-27 26-29 27-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17 18-19

18-23 19-20 20-21 21-22 22-23

exact/norm bonds :

7-9 9-10 10-11 26-29 27-28

exact bonds :

3-24 6-7 7-8 11-13 16-19 24-25 25-26 26-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17 18-19

18-23 19-20 20-21 21-22 22-23

isolated ring systems :

containing 1 : 12 : 18 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS

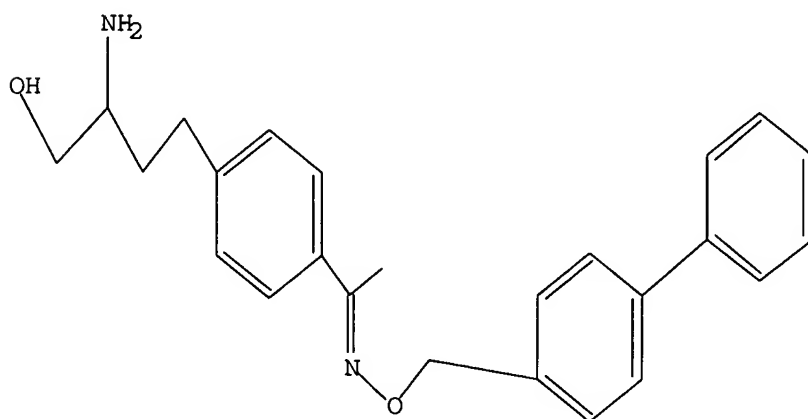
28:CLASS 29:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 10:23:51 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

08/30/2006 10776946.trn

100.0% PROCESSED 2 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:23:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 37 TO ITERATE

100.0% PROCESSED 37 ITERATIONS
SEARCH TIME: 00.00.01

20 ANSWERS

L3 20 SEA SSS FUL L1

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FULL ESTIMATED COST	166.94	167.15

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FILE COVERS 1907 - 30 Aug 2006 VOL 145 ISS 10
FILE LAST UPDATED: 29 Aug 2006 (20060829/ED)

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=> s l3

L4 1 L3

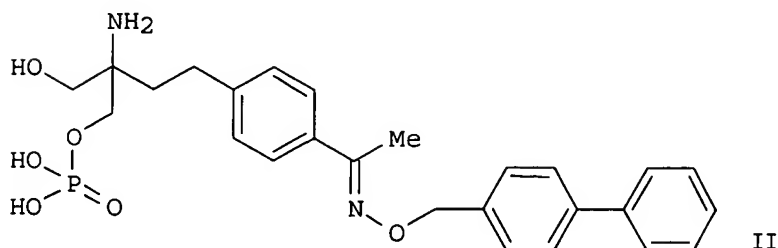
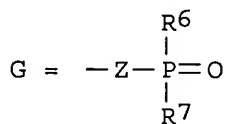
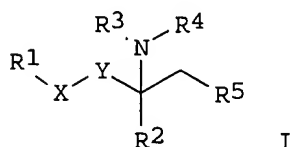
=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:698132 HCAPLUS
DOCUMENT NUMBER: 141:225150
TITLE: Preparation of novel acetophenone oxime derivs. for the treatment of disorders mediated by lymphocyte interactions

08/30/2006 10776946.trn

INVENTOR(S): Pan, Shifeng; Gray, Nathanael; Mi, Yuan; Gao, Wenqi;
Fan, Yi; Hefebvre, Sophie
PATENT ASSIGNEE(S): Icon LLC, Bermuda
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004071442	A2	20040826	WO 2004-US4006	20040211
WO 2004071442	A3	20041028		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004210697	A1	20040826	AU 2004-210697	20040211
CA 2515638	AA	20040826	CA 2004-2515638	20040211
US 2004248952	A1	20041209	US 2004-776946	20040211
EP 1594508	A2	20051116	EP 2004-710227	20040211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004007401	A	20060221	BR 2004-7401	20040211
CN 1761468	A	20060419	CN 2004-80006855	20040211
JP 2006517591	T2	20060727	JP 2006-503494	20040211
PRIORITY APPLN. INFO.:				
			US 2003-446648P	P 20030211
			US 2003-464809P	P 20030421
			US 2003-472012P	P 20030519
			WO 2004-US4006	A 20040211
OTHER SOURCE(S): CASREACT 141:225150; MARPAT 141:225150				
GI				



AB The title compound I [Y = -CH₂CH₂-, -CH₂CH(OH)-, -CH(OH)CH₂-, -C(O)CH₂-, -CH₂C(O)-, -CH=CH-, or 1,2-cyclopropylene; X = arylene or heteroarylene optionally substituted by one to three substituents selected from halo, alkyl, or halo substituted alkyl; R₁ = alkyloxyimino, iminoxyalkyl, isoxazolyl, or oxazolyl; R₂ = H, (halo substituted)(cyclo)alkyl, alkenyl, alkynyl, or alkyl optionally substituted on the terminal C atom by OH or a residue of formula (G); R₃, R₄ = H or alkyl optionally substituted by halo or acyl; R₅ = OH, O-acyl NH-acyl, or a residue of formula (G), Z = O, S, (CH₂)_m (m = 1-2), CF₂ or (substituted)amino; R₆, R₇ = H, OH, (substituted)alkyl, or alkoxy with the proviso that R₆ and R₇ are not both hydrogen] were prepared for the treatment or prevention of diseases or disorders mediated by lymphocyte interactions, particularly diseases associated with EDG/S1P receptor mediated signal transduction. Thus, reaction of phosphoric acid 4-[2-(4-acetyl-phenyl)-ethyl]-2-methyl-4,5-dihydrooxazol-4-ylmethyl ester di-tert-Bu ester (preparation given) with 4-phenylbenzyloxyamine hydrochloride yielded compound II. The latter has an EC₅₀ = 0.86 nM in the EDG-1 (S1P1) GTP [γ -35S] binding assay.

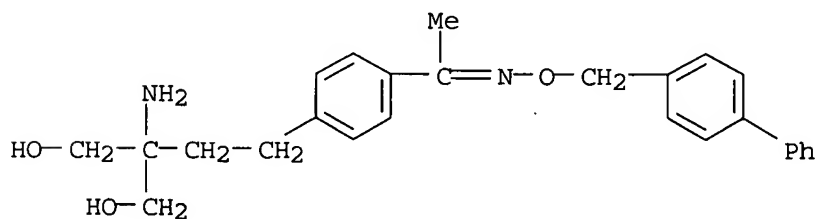
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 745078-50-6P 745078-52-8P 745078-54-0P
 745078-61-9P 745078-62-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel acetophenone oxime derivs. for treatment of disorders mediated by lymphocyte interactions)

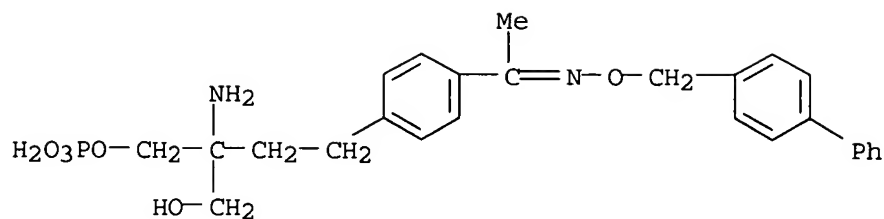
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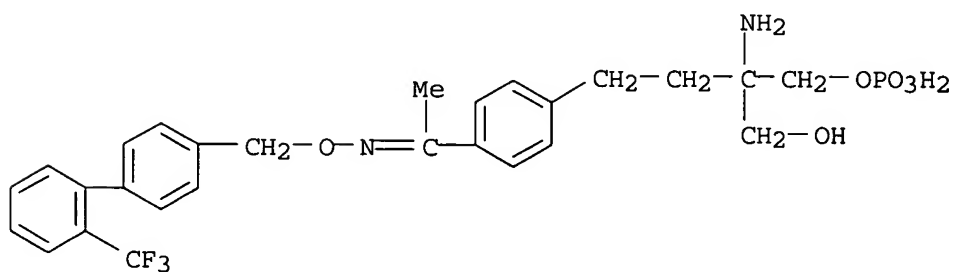
RN 745078-28-8 HCAPLUS

CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-[(phosphonooxy)methyl]butyl]phenyl]-, O-([1,1'-biphenyl]-4-ylmethyl)oxime (9CI) (CA INDEX NAME)



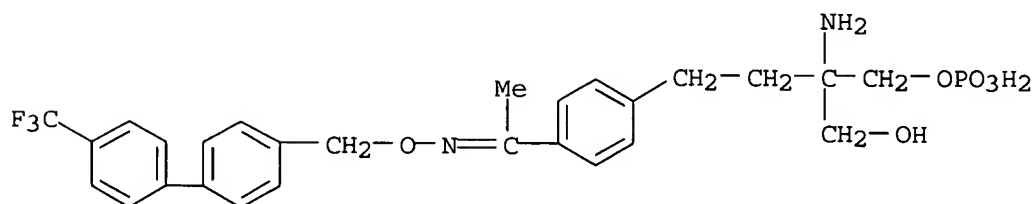
RN 745078-29-9 HCAPLUS

CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-[(phosphonooxy)methyl]butyl]phenyl]-, O-[[2'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)



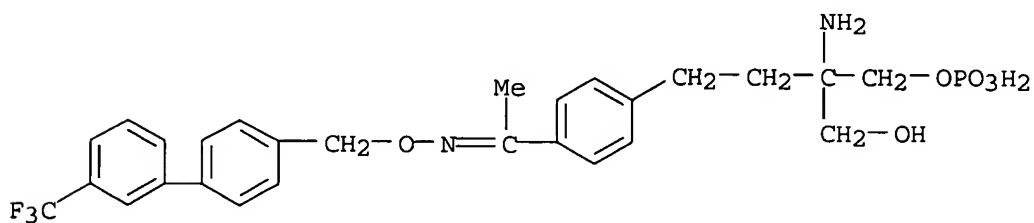
RN 745078-30-2 HCAPLUS

CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-[(phosphonooxy)methyl]butyl]phenyl]-, O-[[4'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)



RN 745078-31-3 HCAPLUS

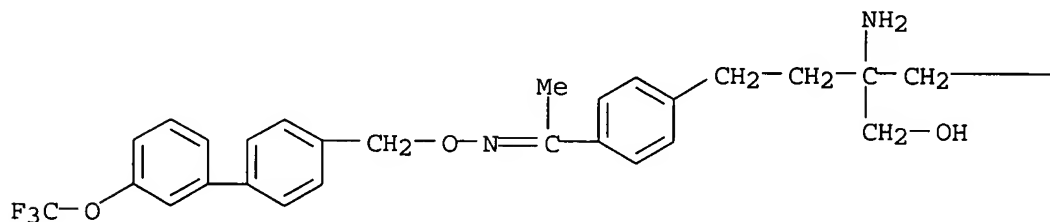
CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-[(phosphonooxy)methyl]butyl]phenyl]-, O-[[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)



08/30/2006 10776946.trn

RN 745078-32-4 HCAPLUS
CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-[(phosphonooxy)methyl]butyl]phenyl]-, O-[[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)

PAGE 1-A

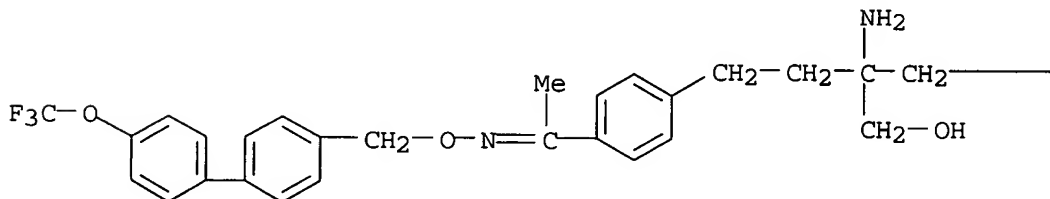


PAGE 1-B

—OPO₃H₂

RN 745078-33-5 HCAPLUS
CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-[(phosphonooxy)methyl]butyl]phenyl]-, O-[[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)

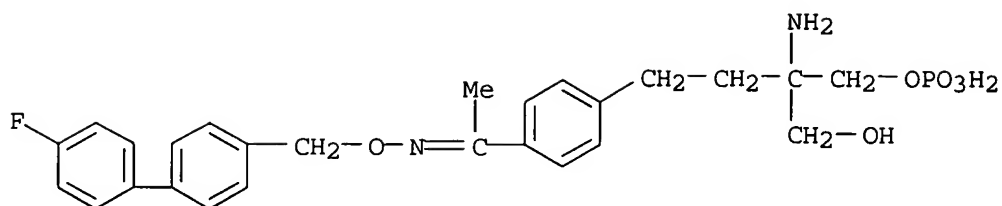
PAGE 1-A



PAGE 1-B

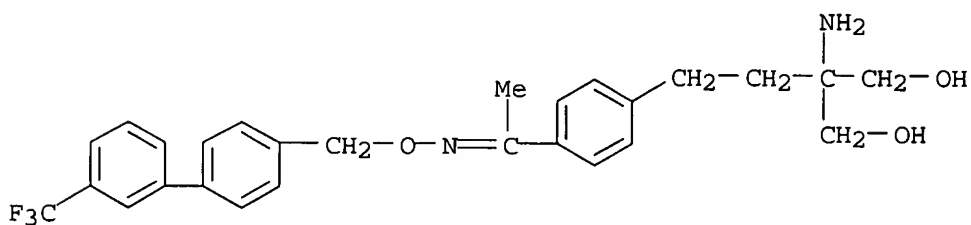
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RN 745078-37-9 HCAPLUS
CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-[(phosphonooxy)methyl]butyl]phenyl]-, O-[[4'-fluoro[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)



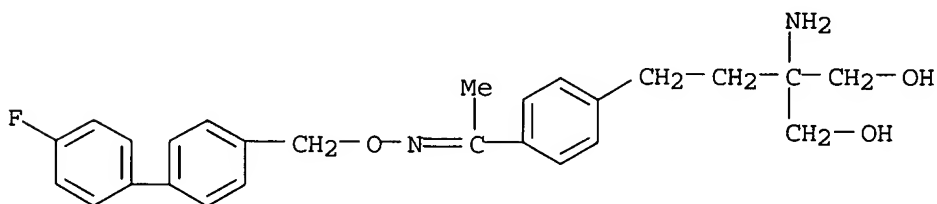
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CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-(hydroxymethyl)butyl]phenyl]-, O-[[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)



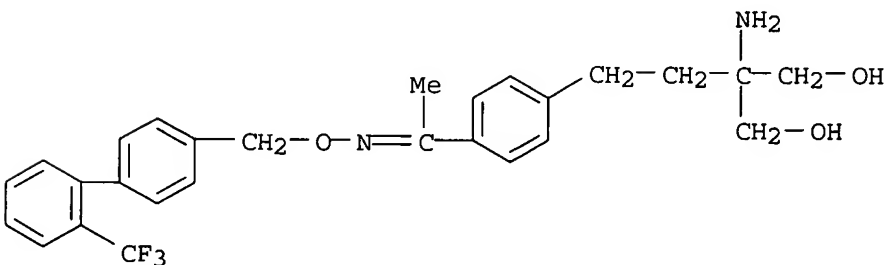
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RN 745078-40-4 HCAPLUS

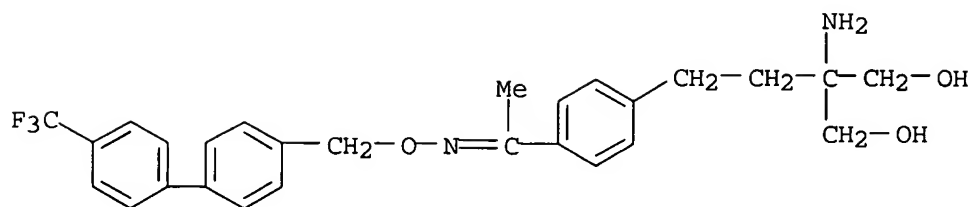
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RN 745078-41-5 HCAPLUS

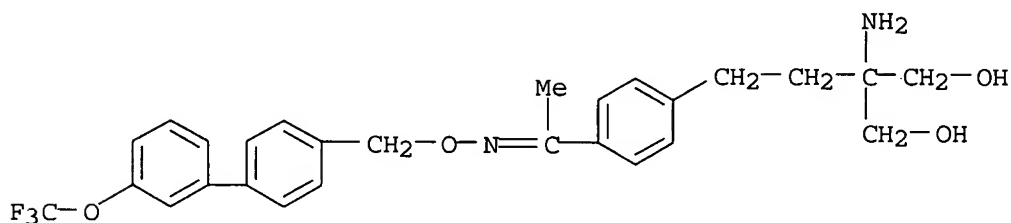
CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-(hydroxymethyl)butyl]phenyl]-,

O-[[4'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)



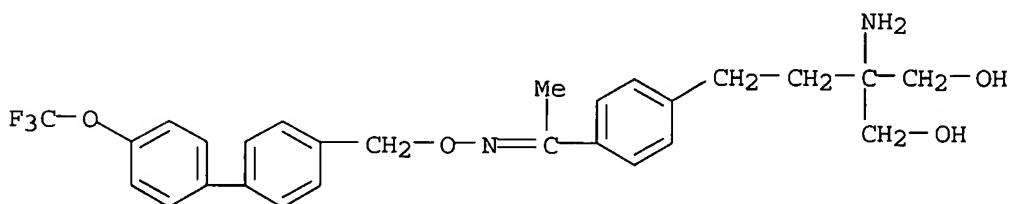
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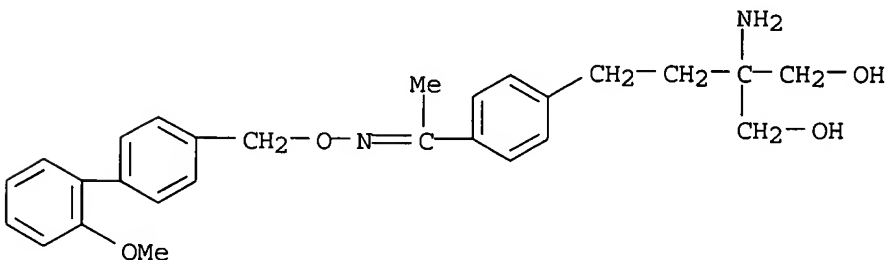
RN 745078-43-7 HCAPLUS

CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-(hydroxymethyl)butyl]phenyl]-, O-[[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]oxime (9CI) (CA INDEX NAME)

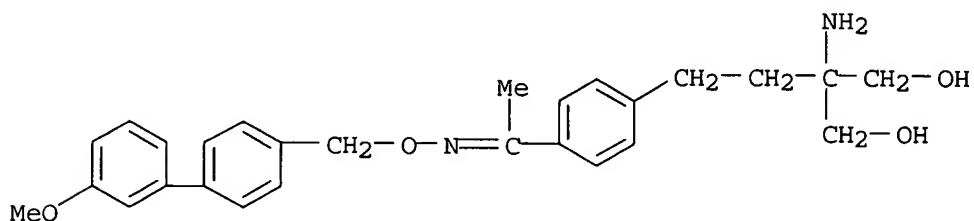


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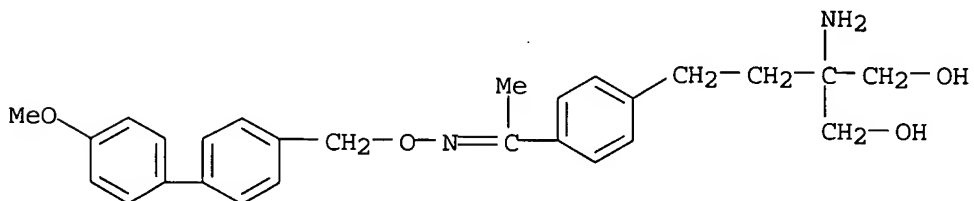
CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-(hydroxymethyl)butyl]phenyl]-, O-[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]oxime (9CI) (CA INDEX NAME)



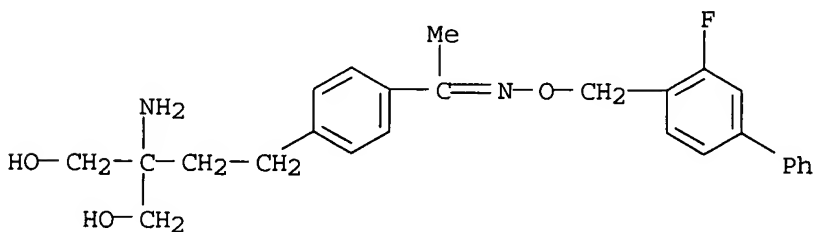
RN 745078-50-6 HCAPLUS

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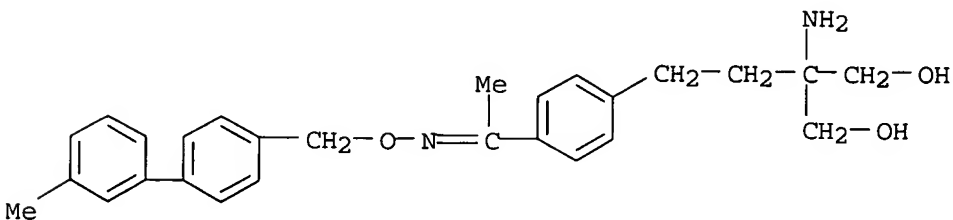
RN 745078-52-8 HCAPLUS

CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-(hydroxymethyl)butyl]phenyl]-,
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RN 745078-54-0 HCAPLUS

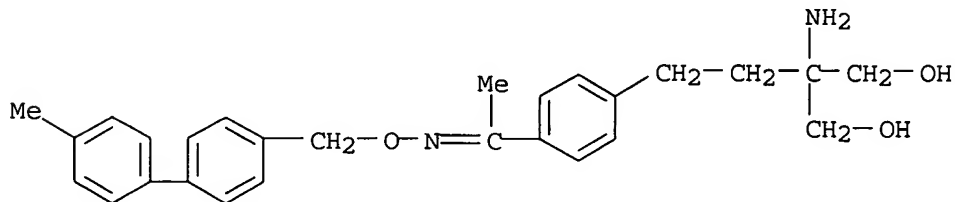
CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-(hydroxymethyl)butyl]phenyl]-,
O-[(3-fluoro[1,1'-biphenyl]-4-yl)methyl]oxime (9CI) (CA INDEX NAME)

RN 745078-61-9 HCAPLUS

CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-(hydroxymethyl)butyl]phenyl]-,
O-[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]oxime (9CI) (CA INDEX NAME)

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RN 745078-62-0 HCAPLUS
CN Ethanone, 1-[4-[3-amino-4-hydroxy-3-(hydroxymethyl)butyl]phenyl]-,
O-[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]oxime (9CI) (CA INDEX NAME)



=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
17.76	184.91

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.75	-0.75

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DICTIONARY FILE UPDATES: 29 AUG 2006 HIGHEST RN 905300-98-3

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

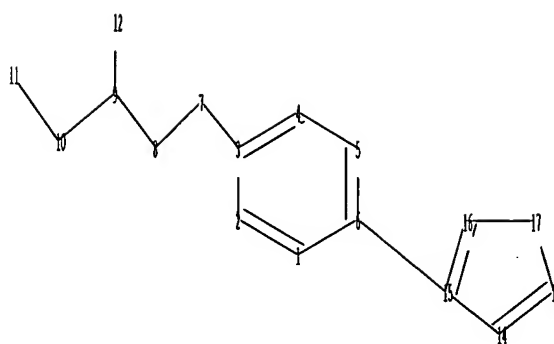
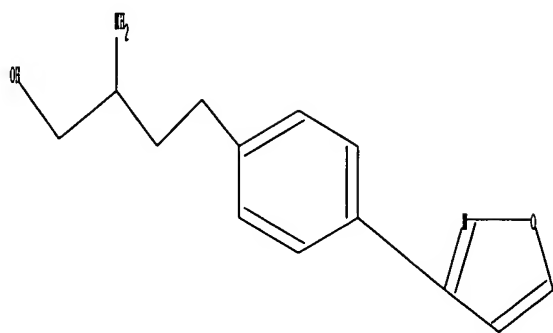
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<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10776946a.str



chain nodes :

7 8 9 10 11 12

ring nodes :

1 2 3 4 5 6 14 15 16 17 18

chain bonds :

3-7 6-15 7-8 8-9 9-10 9-12 10-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-18 15-16 16-17 17-18

exact/norm bonds :

9-12 10-11 15-16

exact bonds :

3-7 6-15 7-8 8-9 9-10 14-15 14-18 16-17 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 :

Match level :

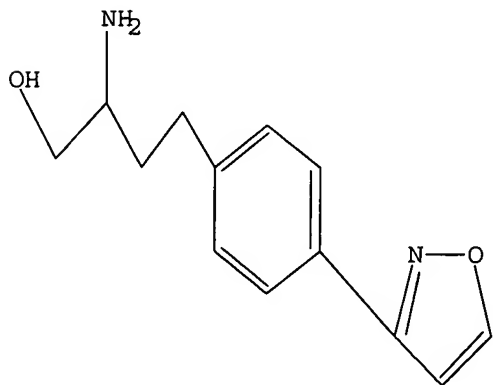
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



08/30/2006 10776946.trn

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 10:27:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 6 TO 266
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 sss full

FULL SEARCH INITIATED 10:27:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 153 TO ITERATE

100.0% PROCESSED 153 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L7 1 SEA SSS FUL L5

=> FIL HCAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	351.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.75

FILE 'HCAPLUS' ENTERED AT 10:27:43 ON 30 AUG 2006

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FILE LAST UPDATED: 29 Aug 2006 (20060829/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17

L8 1 L7

=> d 18 ibib abs hitstr tot

L8 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2003:950770 HCAPLUS
 DOCUMENT NUMBER: 140:4842
 TITLE: Bis-aromatic alkanols
 INVENTOR(S): Pan, Ying; Gao, Wenqi; Gray, Nathanael S.; Hinterding, Klaus; Lefebvre, Sophie; Mi, Yuan; Nussbaumer, Peter; Pan, Shifeng; Wang, Wei; Zecri, Frederic; Perez, Lawrence; Blas, La Montagne, Kenneth Richard; Ettmayer, Peter
 PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.; IRM LLC
 SOURCE: PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003099192	A2	20031204	WO 2003-EP5510	20030526
WO 2003099192	A2	20040318		
WO 2003099192	C1	20050217		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SE, SG, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2486853	AA	20031204	CA 2003-2486853	20030526
AU 2003240714	A1	20031212	AU 2003-240714	20030526
BR 2003011347	A	20050222	BR 2003-11347	20030526
EP 1511473	A2	20050309	EP 2003-730117	20030526
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1655774	A	20050817	CN 2003-812108	20030526
JP 2005527612	T2	20050915	JP 2004-506719	20030526
US 2004048857	A1	20040311	US 2003-445967	20030527
PRIORITY APPLN. INFO.:				
			GB 2002-12210	A 20020527
			GB 2002-26624	A 20021114
			US 2002-432704P	P 20021210
			WO 2003-EP5510	W 20030526

AB A compound of R1XYC(NR3R4)R2CR5 useful for pharmaceutical compns. is prepared wherein Y is -CH2CH2-, -CH2CH(OH)-, -CH(OH)CH2-, -C(O)CH2-, -CH2C(O)-, -CH:CH-, or 1,2-cyclopropylene; X is arylene or C5-6 heteroarylene, R1 is aryl, aryl-C2-4 alkenyl, heteroaryl, or heteroaryl-C2-4 alkenyl; R2 is hydrogen, halogen, C1-4 alkyl, C2-6 alkenyl, C2-6 alkynyl, cycloalkyl, or aryl; each of R3 and R4 is H or C1-4 alkyl; and R5 is H, -OH, -Oacyl, -NHacyl etc. Thus, 6.9 g (2R,5R)-2-[2-(4-benzyloxyphenyl)ethyl]-3,6-diethoxy-5-isopropyl-2-methyl-2,5-dihydropyrazine was treated with 5.17 g tert-butoxycarbonyl anhydride to give Et (R)-4-(4-benzyloxyphenyl)-2-tert-

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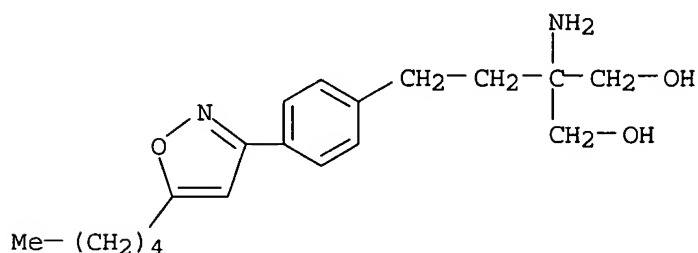
butoxycarbonylamino-2-methylbutyrate, which (2.78 g) was treated with 1,3 mL trifluoromethanesulfonic anhydride to give Et (R)-2-tert-butoxycarbonylamino-2-methyl-4-(4-trifluoromethanesulfonyloxyphenyl)butyrate, which (100 mg) was treated with 75 mg butylboronic acid to give Et (R)-2-tert-butoxycarbonylamino-4-(4'-butylbiphenyl-4-yl)-2-methylbutyrate, which (22 mg) was treated with 20 mg lithium borohydride to give (R)-2-amino-4-(4'-butylbiphenyl-4-yl)-2-methylbutan-1-ol.

IT 628735-13-7P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and characterization of)

RN 628735-13-7 HCAPLUS

CN 1,3-Propanediol, 2-amino-2-[2-[4-(5-pentyl-3-isoxazolyl)phenyl]ethyl]-(9CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.64	359.49

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.75	-1.50

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STN INTERNATIONAL LOGOFF AT 10:28:33 ON 30 AUG 2006